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Full potential KKR approach to the calculation of Hellmann-Feynman force and total energy[1] YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, G.M. STOCKS, Oak Ridge National Laboratory — The Korringa-Kohn-Rostoker (KKR) method is an ab initio electronic structure calculation method based on multiple scattering theory. Unlike the traditional approach, the full-potential KKR method, as well as its linear scaling approach, namely the full-potential LSMS method, does not make a spherical geometry assumption for the LDA potential and the charge density, i.e., the the muffin-tin approximation. Consequently, these full-potential methods allow to calculate the Hellmann-Feynman force acting on each ion in the unit cell. In this presentation, we show an implementation of the full-potential KKR and LSMS methods, discuss the force and total energy calculation in the framework of multiple scattering theory, and finally discuss our approach to overcoming the major computational bottleneck in a full-potential calculation by employing GPGPU acceleration technique.

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Yang Wang
Pittsburgh Supercomputing Center, Carnegie Mellon University

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